

CHANGING YOUR ADDRESS?

In order to receive your journal without interruption, please complete this Change of Address notice and forward to the Publisher, 60 days in advance, if possible.

Old Address: (PLEASE PRINT)

Name _____

Street _____

City _____

State (or Country) _____

Zip Code _____

New Address: (PLEASE PRINT)

Name _____

Street _____

City _____

State (or Country) _____

Zip Code _____

Date New Address Effective: _____

Name of Journal: _____

Plenum Publishing Corporation
233 Spring Street
New York, New York 10013

How To Comply With The New Copyright Law

Participation in the Copyright Clearance Center (CCC) assures you of legal photocopying at the moment of need.

Libraries everywhere have found the easy way to fill photocopy requests legally and instantly, without the need to seek permissions, from more than 3000 key publications in business, science, humanities and social science. You can:

Fill requests for multiple copies, interlibrary loan (beyond the CONTU guidelines), and reserve desk without fear of copyright infringement.

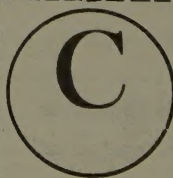
Supply copies from CCC-registered publications simply and easily.

The Copyright Clearance Center is your one-stop place for on-the-spot clearance to photocopy for internal use.

Its flexible reporting system accepts photocopying reports and returns an itemized invoice. You send only one convenient payment. CCC distributes it to the many publishers whose works you need.

And, you need not keep any records, the CCC computer will do it for you. Register now with the CCC and you will never again have to decline a photocopy request or wonder about compliance with the law for any publication participating in the CCC.

To register or for more information, just contact:



Copyright Clearance Center

21 Congress Street
Salem, Massachusetts 01970
(617) 744-3350

a not-for-profit corporation

NAME	TITLE		
ORGANIZATION			
ADDRESS			
CITY	STATE	ZIP	
COUNTRY	TELEPHONE		

Journal of CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH

Volume 19, 1989

Editors

J. L. ATWOOD, University of Alabama, Tuscaloosa, Alabama
S. F. A. KETTLE, University of East Anglia, Norwich, England
M. F. C. LADD, University of Surrey, Surrey, England

Editorial Board

I. BERNAL, University of Houston, Houston, Texas
P. T. BEURSKENS, University of Nijmegen, Nijmegen, The Netherlands
J. C. A. BOEYENS, University of the Witwatersrand, Johannesburg, South Africa
K. BURGER, Attila József University, Szeged, Hungary
M. R. CHURCHILL, State University of New York, Buffalo, New York
A. W. CORDES, University of Arkansas, Fayetteville, Arkansas
W. L. DUAX, Medical Foundation of Buffalo Research Laboratories, Buffalo, New York
M. B. HURSTHOUSE, Queen Mary College, University of London, London, England
B. NORDEN, Chalmers University, Gottenburg, Sweden
C. L. RASTON, Griffith University, Brisbane, Australia
R. D. ROGERS, Northern Illinois University, DeKalb, Illinois
G. A. WEBB, University of Surrey, Surrey, England

Journal of CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH is an international interdisciplinary medium for the rapid publication of research results in the general areas of crystallography and spectroscopy, reporting on new research in crystal chemistry and physics and its relation to problems of molecular structure. The journal publishes papers reporting structural studies of solids, liquids, gases, and solutions, involving spectroscopic, spectrometric, X-ray, electron and neutron diffraction, and theoretical studies. The journal addresses itself not only to crystallographers and spectroscopists, but also to chemists, physicists, biochemists, biologists, and all others who are interested in the results of structural investigations. *JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH* publishes reports of original research as full-length Articles and Notes; it also publishes Book Reviews. All papers will be published in English, and every effort will be made to publish Articles and Notes within six months of the receipt of the manuscript. *JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH* participates in the British Library Document Supply Centre Supplementary Publications Scheme for the deposition of data. It is anticipated that the items deposited will be mainly crystallographic structure factor tables and spectroscopic frequency assignments, in cases where the referees do not recommend their publication. The submission of a manuscript is a representation by its contributors that the manuscript has not been copyrighted, published, or submitted for publication elsewhere. Papers accepted for publication together with data pertaining thereto which are deposited with the British Library Document Supply Centre (see Instructions to Contributors, 10) become the copyright of the publisher. The content of papers is the sole responsibility of the contributors, and publication in *JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH* does not necessarily imply the Editors' and the publisher's concurrence.

JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH is published bimonthly by Plenum Publishing Corporation, 233 Spring Street, New York, N.Y. 10013. Subscription orders should be addressed to the publisher. Advertising inquiries should be addressed to the Advertising Sales Representative, Daniel S. Lipner, Weston Media Associates, P.O. Box 1110, Greens Farms, Connecticut 06436—telephone: (203) 261-2500. *JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH* is abstracted or indexed in Chemical Abstracts, Chemical Titles, Current Contents, Physics Briefs, Referativnyi Zhurnal, Science Citation Index, and Solid State Abstracts Journal. © 1989 Plenum Publishing Corporation. *JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH* participates in the Copyright Clearance Center (CCC) Transactional Reporting Service. The appearance of a code line at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use. However, this consent is given on the condition that the copier pay the flat fee of \$6.00 per copy per article (no additional per-page fees) directly to the Copyright Clearance Center, Inc., 27 Congress Street, Salem, Massachusetts 01970, for all copying not explicitly permitted by Sections 107 or 108 of the U.S. Copyright Law. The CCC is a nonprofit clearinghouse for the payment of photocopying fees by libraries and other users registered with the CCC. Therefore, this consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale, nor to the reprinting of figures, tables, and text excerpts. 0277-8068/89 \$6.00

Subscription rates:

Volume 19, 1989 (6 issues) \$195.00 (outside the U.S., \$225.00).
Volume 20, 1990 (6 issues) \$225.00 (outside the U.S., \$260.00).

Second-class postage paid at New York, N.Y., and at additional mailing offices. Postmaster: Send address changes to *Journal of Crystallographic and Spectroscopic Research*, Plenum Publishing Corporation, 233 Spring Street, New York, N.Y. 10013.

Printed in the USA.

JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH is published bimonthly by Plenum Publishing Corporation, 233 Spring Street, New York, N.Y. 10013. Subscription orders should be addressed to the publisher. Advertising inquiries should be addressed to the Advertising Sales Representative, Daniel S. Lipner, Weston Media Associates, P.O. Box 1110, Greens Farms, Connecticut 06436—telephone: (203) 261-2500. *JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH* is abstracted or indexed in Chemical Abstracts, Chemical Titles, Current Contents, Physics Briefs, Referativnyi Zhurnal, Science Citation Index, and Solid State Abstracts Journal. © 1989 Plenum Publishing Corporation. *JOURNAL OF CRYSTALLOGRAPHIC AND SPECTROSCOPIC RESEARCH* participates in the Copyright Clearance Center (CCC) Transactional Reporting Service. The appearance of a code line at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use. However, this consent is given on the condition that the copier pay the flat fee of \$6.00 per copy per article (no additional per-page fees) directly to the Copyright Clearance Center, Inc., 27 Congress Street, Salem, Massachusetts 01970, for all copying not explicitly permitted by Sections 107 or 108 of the U.S. Copyright Law. The CCC is a nonprofit clearinghouse for the payment of photocopying fees by libraries and other users registered with the CCC. Therefore, this consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale, nor to the reprinting of figures, tables, and text excerpts. 0277-8068/89 \$6.00

Journal of CRYSTALLOGRAPHIC and SPECTROSCOPIC RESEARCH

Volume 19, Number 1, February 1989

Contents

IMPORTANT ANNOUNCEMENT	1
Molecular conformations of γ -lactone rings from crystal structure data. <i>S. A. Thomas and E. B. Agbaji</i>	3
The crystal and molecule structure of three 2,4,6-trinitrobenzene derivatives: α,α,α -trifluoro-2,4,6-trinitrotoluene ($C_7H_2F_3N_3O_6$), 2,4,6-trinitrobenzamide ($C_7H_4N_4O_7$), 2,4,6-trinitrobenzoic acid ($C_7H_3N_3O_8$). <i>Arnold L. Rheingold, Cynthia J. Baldacchini, and Christopher W. Grote</i>	25
Raman spectroscopic studies of gadolinium trichloride as a function of temperature. <i>J. F. Daniel, W. R. Wilmarth, G. M. Begun, and J. R. Peterson</i>	39
X-ray structural investigation of two optically active 1 <i>N</i> -epimers of 2,5,7,10,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-dienenickel(II) diperchlorate. A novel conformation of the macrocyclic ligand. <i>P. Gluziński, R. A. Koliński, J. W. Krajewski, Z. Urbańczyk-Lipkowska, G. D. Andreetti, and G. Bocelli</i>	51
Crystal and molecular structure of diaqua-bis-(3,5-dimethyl-1-guanyl pyrazole) nickel (II) nitrate, $[Ni(C_6N_4H_{10})_2(H_2O)_2](NO_3)_2$. <i>A. Podder, B. P. Mukhopadhyay, N. Saha, A. Saha, and B. Stensland</i>	71
Cobaloxime derivatives: Synthesis and spectroscopic studies of alpha-furilglyoximate of cobalt(III), X-ray structure of bis(thiourea)bis(alpha-furilglyoximate)cobalt(III) nitrate. <i>M. Sakhawat Hussain, H. M. Al-Mohdhar, and E. O. Schlemper</i>	77
Structural and spectroscopic properties of 2-thiophenecarboxaldehyde 2-thienylhydrazone. <i>L. P. Battaglia, A. Bonamartini Corradi, G. Pelosi, and P. Tarasconi</i>	93
Structure of the larvicide <i>N</i> -(2-chlorobenzoyl)- <i>N</i> '-[4-(2-chloro-3,3,3-trifluoroprop-1-enyl)phenyl]urea, $C_{17}H_{11}Cl_2F_3O_2N_2$. <i>Jan C. J. Bart, Mario Calcaterra, Walter Cavigiolo, and Peitro Massardo</i>	99
Studies of systemic acylanilide fungicides: Part V. Crystal structure and molecular conformation of <i>DL</i> -methyl <i>N</i> -(2,6-dimethylphenyl)- <i>N</i> -(2-phenylacetyl)alaninate. <i>J. C. J. Bart, R. Scordamaglia, and M. Calcaterra</i>	109
Crystal structure and vibrational spectra of the methylmercury complex with L-alanine. <i>Marie-Claude Corbeil and André L. Beauchamp</i>	123

Anticancer agent development: X-ray crystal structure and keto-enol tautomerism of dimethyl 1-hydroxy-6,7-methylenedioxy-4-(3',4',5'-trimethoxyphenyl)- <i>trans</i> -3,4-dihydronaphthalene-2,3-dicarboxylate. <i>John R. Peterson, Tamara J. Winter, Hoang D. Do, and Robin D. Rogers</i>	135
A far infrared investigation of anionic species present in solution during the crystallization of a polynuclear bromocuprate(I) cluster containing three-coordinated copper(I). <i>Staffan Andersson, Mikael Håkansson, and Susan Jagner</i>	147
Nitrogen NMR studies on some fused ring <i>N</i> -heterocycles. <i>L. Stefaniak, M. Witanowski, U. Mahmoud, J. D. Roberts, and G. A. Webb</i>	159
X-ray crystallographic determination of the structure and conformation of 7-(1-acetoxy-1-methylethyl)-4a-methyl-octahydro-2(³ H)-naphthalenone. <i>T. Głowiak, C. Hebda, and J. Szykuła</i>	167
The <i>N,N</i> -diacetylaminobenzene group in the structure of 6-methyl-8- <i>N,N</i> -diacetylamino-2,4-bis(trichloromethyl)-1,3-benzodioxin. <i>Anne Irving and Harry M. N. H. Irving</i> ...	175
Disorder arising from the location of enantiomers in a twist-boat structure: 2,6- <i>trans</i> -2,4,6-tris(trichloromethyl)-1-oxa-3,5-dithian. <i>Anne Irving and Harry M. N. H. Irving</i>	183
Crystal and molecular structure of 17- β -methyl- α -isolupanine <i>N</i> (16)-oxide perchlorate monohydrate. <i>A. Katrusiak and Z. Kałuski</i>	193
Crystal structure of copper(II)mellitate, [Cu _{3.5} C ₆ (COO) ₅ (COOH)(OH) ₂ (H ₂ O) _{8.5}] · 4.5H ₂ O. <i>Hatsue Tamura, Kazuhide Ogawa, and Wasuke Mori</i>	203
NOTES	
Crystal and molecular structure of <i>S</i> -(+)-ethyl-O-(4-phenylbenzoyl)lactate, C ₁₈ H ₁₈ O ₄ . <i>W. H. Laarhoven, W. J. C. Prinsen, H. Behm, W. P. Bosman, and Paul T. Beurskens</i>	215
Crystal and molecular structure of (4 <i>R</i> *,5 <i>S</i> *)-5-(3,5-dinitrophenylcarbonyloxy)-4-methoxy-4-methyl-2-cyclopenten-1-one, C ₁₄ H ₁₂ O ₈ N ₂ . <i>A. M. M. Houwen-Claassen, A. J. H. Klunder, H. Behm, F. G. Moers, Paul T. Beurskens, D. Heydenrijk, and H. Schenk</i>	223
ERRATUM	231
INSTRUCTIONS TO CONTRIBUTORS	233

Journal of CRYSTALLOGRAPHIC and SPECTROSCOPIC RESEARCH

Volume 19, Number 2, April 1989

Contents

Crystal and molecular structure of 4,17a-methyl-4,17a-diaza-5 α -androstane (HS353): An intermediate in the design of azasteroid neuromuscular blocking agents. <i>Tapan K. Chattopadhyay, Rex A. Palmer, Harkishan Singh, and Darham Paul</i>	237
(-)-S-Benzyl- α -hydroxymethylcysteine: Confirmation of its (S)-configuration by x-ray analysis of its N-benzoyl derivative. <i>Wanda Wieczorek, Maria Bukowska-Strzyewska, Aleksandra Olma, and Mirosław T. Leplawy</i>	257
Crystal and molecular structure of 4-bromo-2,2,3,3-tetramethyl-1-benzyl-1-phenylphosphetanium bromide. <i>Mazhar-Ul-Haque, William Horne, Sheldon E. Cremer, Paul W. Kremer, and Pawel K. Kafarski</i>	267
Synthesis and structure of 1-(2-amino)phenyl-2-12H-indolo[3,2-c]carbazole ethylacetate solvate, a new indolocarbazole compound. <i>Paolo Domiano, Vittorio Bocchi, and Gerardo Palla</i>	277
Crystal and molecular structure of 4-aminoacetyl-N-p-nitrophenylsulfanilamide. <i>M. Ghosh, A. K. Basak, S. K. Mazumdar, and B. Sheldrick</i>	289
Crystal structure of <i>trans</i> -[PtCl ₂ (Me ₂ PhP)(<i>cis</i> -2,5-dimethylpyrrolidine)]. <i>F. Bachechi and L. Zambonelli</i>	299
Molecular and crystal structure of 1,4-diacethoxynaphthalene: Structural analysis of methyl substituted 1,4-diacethoxynaphthalenes. <i>José Gonzalo Rodríguez, Alfonso de Pablo, Julian Lopez de Lerma, and Aurea Perales</i>	307
Crystal and molecular structure of 3,3-diphenyl-3-phosphoniabicyclo[3.2.1]oct-6-ene bromide monohydrate. <i>Mazhar-Ul-Haque, William Horne, Sheldon E. Cremer, and James T. Most</i>	317
On the stereochemistry of lignin model compounds of the arylglycerol- β -aryl ether type: Crystal structure of <i>erythro</i> -1-(4-hydroxy-3,5-dimethoxyphenyl)-2-(4-hydroxy-methyl-2,6-dimethoxyphenoxy)-1,3-propanediol, C ₂₀ H ₂₆ O ₉ . <i>Rolf Stromberg and Knut Lundquist</i>	331
Structural investigation on hexasubstituted benzene derivatives. Part 2: The structure of meta-dinitrotetramethylbenzene and molecular mechanics analysis on meta and ortho derivatives. <i>Ottorino Ori, Paolo Sgarabotto, Franco Ugozzoli, and Salvatore Sorriso</i>	341
Structure and IR spectroscopic behavior of 2,4-dimethylpyridinium pentachlorophenolate. <i>I. Majerz, Z. Malarski, and T. Lis</i>	349

Crystal structures of 4-amino-1,2,4-triazolidine-3,5-dione (urazine) ($C_2H_4N_4O_2$) and dichlorobis(4-amino-1,2,4-triazolidine-3,5-dione- <i>N,O</i>)copper(II) ($C_4H_8Cl_2CuN_8O_4$). <i>Francesco Bigoli, Maurizio Lanfranchi, and Maria Angela Pellinghelli</i>	357
Crystal and molecular structure of inner-chelate <i>trans</i> -1,4,10,13-tetraoxa-7,16-diazacyclooctadecane-7,16-diacetatozinc(II), $C_{16}H_{28}N_2O_8Zn$. <i>P. Gluziński, J. W. Krajewski, R. A. Koliński, Z. Urbańczyk-Lipkowska, A. Mishnyov, and A. Kemme</i> ..	369
Crystal and molecular structure of chloramphenicol analog: 2-amino-4-methoxy-2',2'-dichloroacetophenone. <i>Amitabha De, Yoshiki Matsuura, and Masami Kusunoki</i>	379
Crystal and molecular structure of 1,4,10-trioxa-7,13-diaza-cyclopentadecane-7,13-diacetatozinc(II) dihydrate, $C_{14}H_{24}N_2O_7Cu \cdot 2H_2O$. <i>Z. Urbańczyk-Lipkowska, P. Gluziński, J. W. Krajewski, R. A. Koliński, A. Kemme, and A. Mishnyov</i>	387
Molecular structure and electronic populations of two ligands for the benzodiazepine receptor sites: 3-methyl-6-phenyl- and 3-methyl-7-phenyl-1,2,4-triazolo[4,3- <i>b</i>]pyridazines, SR95199 and SR95195; x-ray diffraction analysis and <i>ab initio</i> MO calculations. <i>Thierry Boulanger, Laurence Ledent, Bernadette Norberg, Daniel P. Vercauteren, Guy Evrard, and François Durant</i>	399
INSTRUCTIONS TO CONTRIBUTORS	411

Journal of CRYSTALLOGRAPHIC and SPECTROSCOPIC RESEARCH

Volume 19, Number 3, June 1989

Contents

The crystal and molecular structure of 14- β -N-pentylaminomorphinone, $C_{22}H_{28}N_2O_3$. <i>S. M. Evans, E. F. Ezell, and S. J. Sondheimer</i>	415
Alkylation of tellurium tetrachloride by trimethylaluminum. Synthesis and molecular structure of $[Te(CH_3)_3][Al(CH_3)_2Cl_2]$: A novel organotelluronium-aluminum oligomer. <i>Samuel A. Sangokoya, William T. Pennington, and Gregory H. Robinson</i>	433
Structures of NN' -ethylenebis(monothioacetylacetoneiminato)nitrosylcobalt and NN' -ethylenebis(2-hydroxyacetophenoneiminato)nitrosylcobalt. <i>L. F. Larkworthy, D. C. Povey, G. W. Smith, and B. J. Tucker</i>	439
Relating infra red spectral data to structure for a series of $M_2(CO)_{10-n}(L)_n$ complexes ($M = Re, Mn$; $L = CNR, PR_3$; $R = Alkyl, Aryl$; $n = 1 - 4$). <i>Gillian W. Harris and Neil J. Coville</i>	451
Crystal and molecular structure of <i>bis</i> (<i>o</i> -phenylenethiourea)selenium(II)chloride dihydrate, $C_{14}H_{12}N_4S_2Cl_2Se \cdot 2H_2O$. <i>Sp. Chidambaram, G. Aravamudan, V. Ganesh, M. Seshasayee, T. A. Sibanova, B. V. Merinov, and V. I. Simonov</i>	465
Crystal structure of DMAP-C-HMTCAQ, $C_{30}H_{20}N_6O_2$, <i>N,N</i> -dimethylaminophenyl-carbamate-2'-hydroxymethyl-11,11,12,12-tetracyano-anthraquinodimethan. <i>R. M. Metzger, R. K. Laidlaw, E. Torres, and C. A. Panetta</i>	475
Steroids and related studies, part 75: The crystal and molecular structure of 17 α -(2-hydroxyethyl)-17 α -aza-D-homo-5-androsten-3 β ol(HS407). <i>Rex A. Palmer, Tapan K. Chattopadhyay, Harkishan Singh, and Dharam Paul</i>	483
The crystal structure of $UO_2Cl_2(OH_2)(MeCN)_2 \cdot 2MeCN$. <i>Tom J. Hall, Carol J. Mertz, Steven M. Bachrach, William G. Hipple, and Robin D. Rogers</i>	499
Crystal and molecular structure of 3-(4-chlorobenzoylimino)-5,6-dihydro-3H-imidazo [2,1-c]-1,2,4-dithiazole. <i>Maria Gdaniec, Krzysztof Osmialowski, and Franciszek Sączewski</i>	507
Synthesis, structural, and spectroscopic study of rhenium(III) and rhenium(V) 4,6-dimethylpyrimidine-2-thiolate/triphenylphosphine mixed complexes: Crystal and molecular structure of $[ReCl_2(pymS)(PPh_3)_2] \cdot C_3H_6O$ and $[ReOCl_2(pymS)(PPh_3)]$. <i>R. Battistuzzi, T. Manfredini, L. P. Battaglia, A. Bonamartini Corradi, and A. Marzotto</i>	513

2 α -Hydroxy-3 α -[N-alkyl(aryl)]pinanoamines. Part I. Preparation and nature of some Schiff bases of 2 α -hydroxypinan-3-one. Crystal and molecular structure of α -hydroxy-2,6,6-trimethylbicyclo[3.1.1]hepta-3-ylidenaminobenzene. Stanisław Wojciech Markowicz, Janina Karolak-Wojciechowska, and Witold Kwiatkowski	535
Crystal and molecular structure of 6-chloro-3-cyclopentylmethyl-3,4-dihydro-7-sulfamyl-2H-1,2,4-benzothiadiazine-1,1-dioxide. A. K. Basak, M. Ghosh, S. K. Mazumdar, and S. Chaudhuri	547
Structure of 3 α ,12 β -dihydroxy-2 β -morpholino-5 α -pregnan-20-one, C ₂₅ H ₄₁ O ₄ N. Zdzisław Gałdecki, Paweł Grochulski, Zdzisław Wawrzak, William L. Duax, and Phyllis D. Strong	561
Structure of 9 α ,11 β -dichloro-4-pregnene-3,20-dione, C ₂₁ H ₂₈ O ₂ Cl ₂ . Zdzisław Gałdecki, Paweł Grochulski, Zdzisław Wawrzak, William L. Duax, and Phyllis D. Strong	569
Structure of 17 α -methyl-testosterone semihydrate, C ₂₀ H ₃₀ O ₂ · $\frac{1}{2}$ H ₂ O. Zdzisław Gałdecki, Paweł Grochulski, and Zdzisław Wawrzak	577
Structure of crystal violet tetraphenylborate. Brenda D. Spangler, Petr Vanýsek, Irma C. Hernandez, and Robin D. Rogers	589
NOTES	
Crystal and molecular structure of lapachenole. Joseph H. Reibenspies, Howard J. Willams, Claudio Ortiz, A. Ian Scott, Mauricio Suarez, and Xorge A. Dominguez ..	597
Crystal and molecular structure of four compounds resulting from nucleophilic addition of 2H-pyrroles to dimethyl acetylene-dicarboxylate, methyl propiolate and phenyl isocyanate. A. Boukhari, A. Eddaif, A. Laurent, P. Mison, and R. Faure	603
ERRATUM	623
INSTRUCTIONS TO CONTRIBUTORS	625

Journal of CRYSTALLOGRAPHIC and SPECTROSCOPIC RESEARCH

Volume 19, Number 4, August 1989

Contents

Steroids and related studies, Part 76: Crystal and molecular structure of 4,17a-di(2-hydroxyethyl)-4,17a-diaza-D-homo-5 α -androstande (HS461). <i>Rex A. Palmer, A. I. El-Shora, Harkishan Singh, and Dharam Paul</i>	629
Crystal and molecular structure of 5-carbamyl-5H-dibenzo[b, f] azepine. <i>John N. Lisgarten, Rex A. Palmer, and Jose W. Saldanha</i>	641
1,4-Benzodiazepines as ligands. Synthesis, characterization and crystal and molecular structure of bis(8-chloro-6-(o-chlorophenyl)-1-methyl-4H-s-triazolo[4,3-a]1,4-benzodiazepine (triazolam)) cadmium (II) dichloride. <i>Adriano Benedetti, Antonio C. Fabretti, and Carlo Preti</i>	651
Geometric alignment in the structure of 6,8-dichloro-2-trichloromethyl-4-dichloromethylene-1,3-benzodioxin consistent with incipient <i>cis</i> -elimination of HCl. <i>Anne Irving and Harry M. N. H. Irving</i>	661
Vibrational spectra and thermodynamic properties of 2,4,6-tribromobenzonitrile. <i>J. A. Faniran</i>	671
A comparative UV vapor-phase photoelectron study of substituted styrenes and phenylacetylenes. <i>David Ajò, Eugenio Tondello, Franco Marcuzzi, and Giorgio Modena</i>	683
Crystal structure of racemic 5-(p-nitrobenzoylamino)-5-methyl-4-oxo-1,3-dioxane. <i>Marek L. Glówka, Zbigniew J. Kamiński, Valerio Bertolasi, and Gastone Gilli</i>	695
Crystal structure of 7-cyano-6,7-dimethyl-1-phenyl-1,3,6,7-tetrahydro-2,1-benzoxaphospole 1-oxide. <i>Marek L. Glówka, Henryk Krawczyk, Ryszard Bodalski, and Valerio Bertolasi</i>	701
Crystal structure of bis(benzimidazolium) tetrabromocuprate(II). <i>A. Tosik and M. Bukowska-Strzyżewska</i>	707
Crystal structures of dimethylsuccinate and dimethyloxalate: Carbonyl group orientation for C ¹³ chemical shielding tensor studies. <i>G. P. Jones, B. A. Cornell, E. Horn, and E. R. T. Tiekink</i>	715
Crystal and molecular structure of voacangine: An alkaloid from <i>Stemmadenia Donnell-Smithii</i> . <i>M. Soriano-García, A. Rodríguez, F. Walls, and R. Toscano</i>	725

Crystal structure of the diacetate of (+)-epipinoresinol, $C_{24}H_{26}O_8$. <i>Knut Lundquist and Rolf Stomberg</i>	733
A novel mixed valence iodide bridged Te(II)–Te(IV) complex featuring diisopropyldithiocarbamate(L) and iodide: $ILTe^{II}(I)Te^{IV}L_2I$. <i>V. Ganesh, M. Seshasayee, V. Kumar, Sp. Chidambaram, G. Aravamudan, K. Goubitz, and H. Schenk</i>	745
Synthesis, spectroscopic studies, and crystal structure of theophyllinium tetrabromopalladate(II). <i>J. M. Salas, E. Colacio, M. N. Moreno, J. Ruiz, T. Debaerdemaeker, J. Via, and M. I. Arriortua</i>	755
NOTES	
Crystal and molecular structure of <i>p</i> -chlorothymols, I: 4-chloro-2-isopropyl-5-methylphenol (PCNT). <i>S. Rantsordas and M. Perrin</i>	765
Crystal structure of a decahydroquinoline thiocarbamate derivative (SR33434) with anticalcic properties. <i>Veronique Gibon, Sylvia Blesgen, Guy Evrard, and François Durant</i>	775
INSTRUCTIONS TO CONTRIBUTORS	787

Journal of CRYSTALLOGRAPHIC and SPECTROSCOPIC RESEARCH

Volume 19, Number 5, October 1989

Contents

X-ray structure determination of cyclobutane photodimers from (Z)- α,β -diarylacrylonitriles. <i>Maria E. Amato, Giuseppe Musumarra, Giuseppe Scarlata, Dorian Lamba, and Riccardo Spagna</i>	791
Complexation with diol host compounds. Part 2. Structures of 1,1,2,2-tetraphenylethane-1,2-diol and its 1:2 molecular inclusion complex with dimethylsulphoxide. <i>Dianne R. Bond, Susan A. Bourne, Luigi R. Nassimbeni, and Fumio Toda</i>	809
X-ray structure and UV spectroscopic studies of (adeninato-N9)triethylphosphinegold(I). <i>Edward R. T. Tiekink, Tomas Kurucsev, and Bernard F. Hoskins</i>	823
Crystal structure of 1,3-(N,N'-benzamide)-2-methyl-1-pentene. <i>Gabriele Bocelli</i>	841
Complexation with diol host compounds. Part 3. Molecular inclusion of 4-methylcyclohexanone and 2-methylcyclohexanone by the host, <i>trans</i> -9,10-dihydroxy-9,10-diphenyl-9,10-dihydroanthracene. <i>Dianne R. Bond, Luigi R. Nassimbeni, and Fumio Toda</i>	847
Studies in molecular structure and conformation of aminophosphonic acids: Crystal and molecular structure of <i>N</i> -phosphonomethyl-L-threonine. <i>W. Sawka-Dobrowolska, T. Glowiak, and J. Barycki</i>	861
Crystal structure and spectroscopic study of 2-(<i>p</i> -methoxycarbonylphenyl)-1,3,5,5,7,8,8-heptamethyl-2,4,5,6,7,8-hexahydroindeno[1,2- <i>c</i>]-pyrrole-7-carbonitrile. <i>F. Camps, J. Coll, C. Mola, J. Rius, E. Molins, and C. Miravittles</i>	873
Crystal and molecular structure of 1-(2-isopropylcarbomoylpropan-2-ylamino) 3-(1-naphthoxy)propan-2-ol ($C_{26}H_{28}N_2O_3$). <i>M. W. Wiczorek, G. D. Bujacz, E. Galas, J. Zjawiony, and A. Wojciechowska</i>	883
2- α -Hydroxy-3 α -[<i>N</i> -alkyl(aryl)]-pinanoamines. Part II. Synthesis and the nature of some pinanoamines and crystal and molecular structure of 2 α -hydroxy-3 α -(<i>N</i> - <i>n</i> -butyl)-pinanoamine hydrochloride. <i>Janina Karolak-Wojciechowska, Witold Kwiatkowski, and Stanislaw Wojciech Markowicz</i>	893
Structural Investigation on hexasubstituted benzene derivatives. Part 1. The structure of ortho-dinitrotetramethylbenzene. <i>Paolo Sgarabotto, Franco Ugozzoli, and Salvatore Sorriso</i>	905

Preparation and electron spin resonance study of copper(II) complexes with sugar type ligands. <i>L. Nagy, L. Zsikla, K. Burger, A. Rockenbauer, and J. T. Kiss</i>	911
---	-----

NOTE

On the absolute configuration of the synthetic macrolide patulolide <i>C. Gezina Beurskens, J. M. M. Smits, Paul T. Beurskens, L. Thijs, D. M. Egenberger, and B. Zwanenburg</i>	919
--	-----

INSTRUCTIONS TO CONTRIBUTORS	925
------------------------------------	-----

Journal of CRYSTALLOGRAPHIC
and SPECTROSCOPIC RESEARCH

Volume 19, Number 6, December 1989

Contents

The crystal field theory for D_{2d} symmetric complexes and the splitting of d-orbitals of Mo^{5+} in $Mo[S_2CN(C_2H_5)_2]_4I_3$. *Yang Jian-Hua and Zhou Kang-Wei* 929

Structure of 17β -hydroxy-1-4-androstadien-3-one monohydrate $C_{19}H_{26}O_2 \cdot H_2O$.
Zdzisław Gałdecki, Paweł Grochulski, Zdzisław Wawrzak, and Andrzej Szczepkowski .. 933

Structure of 17β -hydroxy-4-pregnen-20-yn-3-one, $C_{21}H_{38}O_2$. *Zdzisław Gałdecki, Paweł Grochulski, Zdzisław Wawrzak, and William L. Duax* 941

Structure of 6β -acetyoxyprogesterone, $C_{23}H_{32}O_4$. *Zdzisław Gałdecki, Paweł Grochulski, Zdzisław Wawrzak, and William L. Duax* 949

Di- μ -sulphido-bis[4-methyl-piperidine-dithiocarbamate tin(IV)]: Synthesis, characterization, and crystal and molecular structure. *Antonio C. Fabretti and Carlo Preti* 957

Crystal and molecular structures of 1-(2-iso butyl-yl-carbamoyl propan-2-ylamino) 3-(1-naphthoxy)propan-2-ol hydrochloride (1) ($C_{21}H_{31}N_2O_3Cl$) and 1-(2-isobutyloxycarbonylo propan-2-ylamino) 3-(1-naphthoxy)propan-2-ol hydrochloride (2) ($C_{21}H_{30}NO_4Cl$). *M. C. Wieczorek, G. D. Bujacz, E. Galas, J. Zjawiony, and A. Wojciechowska* 967

Structure of progesterone hydroquinone monohydrate (1:1:1), $C_{21}H_{30}O_2 \cdot C_6H_6O_2 \cdot H_2O$. *Zdzisław Gałdecki, Paweł Grochulski, Zdzisław Wawrzak, and William L. Duax* 983

Synthesis and UV photoelectron investigation of the "peptide units" of α,β -dehydroamino acids. *J. A. Mayoral, C. Cativiela, M. P. Lopez, D. Ajò, and F. De Zuane* 993

$A^{13}C$ and ^{15}N NMR study of some furoxans and related compounds. *B. Kamiński, W. Schilf, J. Sitkowski, L. Stefaniak, and G. A. Webb* 1003

Crystal and molecular structure of phenylbenzyl-1-(2,2,3-trimethylcyclopropyl)phosphine oxide. *Mazhar-Ul-Haque, Jamil Ahmed, William Horne, Sheldon E. Cremer, Paweł K. Kafarski, and Paul W. Kremer* 1009

Crystal and molecular structure of the ruthenium-carbene-tetraborohydrate complex $[Ru(BH_4)(L^{Ar})(PPh_3)_2]$; ($L^{Ar} = CN(C_6H_4Me-4)CH_2CH_2NC_6H_3Me-4$). *S. A. Thomas* 1017

NOTE

Crystal and molecular structure of [dicarbonyl(η -cyclopentadienyl)ferrio]triphenylarsine tetrafluoroborate, $[(C_6H_5)_3As\{Fe(CO)_2(C_5H_5)\}] [BF_4]$. *H. Schumann, J. M. M. Smits, and Paul T. Beurskens* 1033

AUTHOR INDEX TO VOLUME 19 1041

INSTRUCTIONS TO CONTRIBUTORS 1057

